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NEWS 14 APR 18 New CAS Information Use Policies available online
NEWS 15 APR 25 Patent searching, including current-awareness alerts (SDIs), based on application date in CA/CAplus and USPATFULL/USPAT2 may be affected by a change in filing date for U.S. applications.
NEWS 16 APR 28 Improved searching of U.S. Patent Classifications for U.S. patent records in CA/CAplus
NEWS 17 MAY 23 GBFULL enhanced with patent drawing images
NEWS 18 MAY 23 REGISTRY has been enhanced with source information from CHEMCATS
NEWS 19 JUN 06 STN Patent Forums to be held in June 2005
NEWS 20 JUN 06 The Analysis Edition of STN Express with Discover! (Version 8.0 for Windows) now available
NEWS 21 JUN 13 RUSSIAPAT: New full-text patent database on STN
NEWS 22 JUN 13 FRFULL enhanced with patent drawing images
NEWS 23 JUN 20 MEDICONF to be removed from STN
NEWS 24 JUN 27 MARPAT displays enhanced with expanded G-group definitions and text labels

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

| | |
|------------|---|
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| NEWS LOGIN | Welcome Banner and News Items |
| NEWS PHONE | Direct Dial and Telecommunication Network Access to STN |
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10/774,619

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 JUN 2005 HIGHEST RN 853295-05-3
DICTIONARY FILE UPDATES: 29 JUN 2005 HIGHEST RN 853295-05-3

New CAS Information Use Policies. enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

* The CA roles and document type information have been removed from *

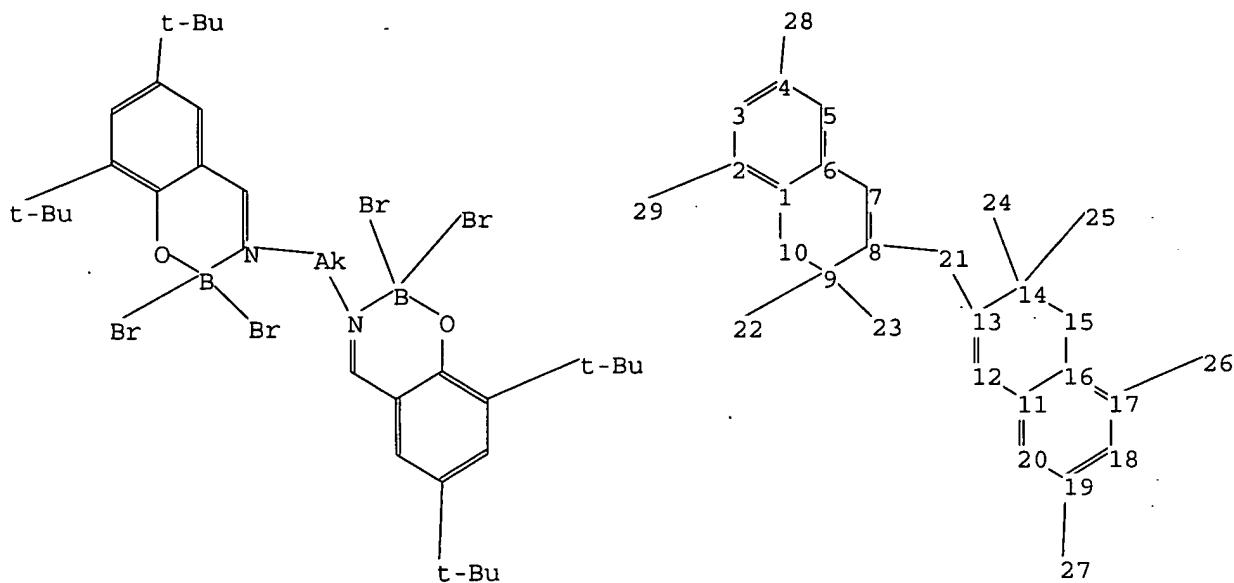
* effective March 20, 2005. A new display format, IDERL, is now *
the IBS catalog display format and will be used throughout the system.

* available and contains one or more blank lines.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer

to the file summary sheet on the web at:

=>
Unloading C:\Program Files\Sympy\Queries\10774619.str



chain nodes :

21 22 23 24 25 26 27 28 29

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

2-29 4-28 8-21 9-22 9-23 13-21 14-24 14-25 17-26 19-27

ring bonds :

1-2 1-6 1-10 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 11-12 11-16 11-20 12-13
13-14 14-15 15-16 16-17 17-18 18-19 19-20

exact/norm bonds :

1-10 6-7 7-8 8-9 8-21 9-10 11-12 12-13 13-14 13-21 14-15 15-16

exact bonds :

2-29 4-28 9-22 9-23 14-24 14-25 17-26 19-27

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-16 11-20 16-17 17-18 18-19 19-20

isolated ring systems :

containing 1 : 11 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom

20:Atom 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS

28:CLASS 29:CLASS

L1 STRUCTURE UPLOADED

=> S 11

SAMPLE SEARCH INITIATED 17:26:36 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

10/774,619

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 ful
FULL SEARCH INITIATED 17:26:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

L3 5 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
161.33 161.54

FILE 'CAPLUS' ENTERED AT 17:26:48 ON 30 JUN 2005
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FILE COVERS 1907 - 30 Jun 2005 VOL 143 ISS 1
FILE LAST UPDATED: 29 Jun 2005 (20050629/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13
L4 2 L3

=> d 14 ibib hitstr abs 1-2

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:49058 CAPLUS
DOCUMENT NUMBER: 139:149666
TITLE: Dealkylation with boron bromide chelates
AUTHOR(S): Keizer, Timothy S.; De Pue, Lauren J.; Parkin, Sean;
Atwood, David A.

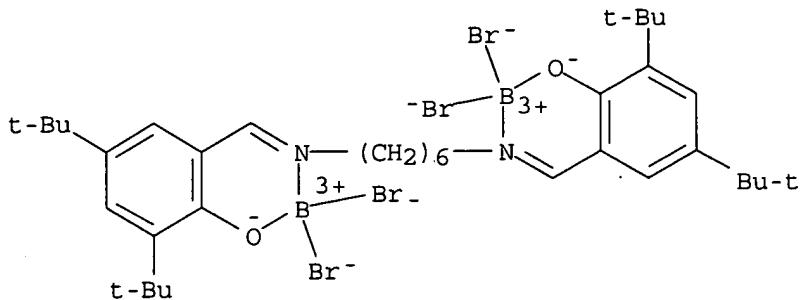
CORPORATE SOURCE: Department of Chemistry, University of Kentucky,
Lexington, KY, 40506-0055, USA
 SOURCE: Journal of Organometallic Chemistry (2003), 666(1-2),
103-109
 CODEN: JORCAI; ISSN: 0022-328X
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:149666

IT 570414-19-6P

RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (mol. structure, phosphate dealkylation; preparation, structure and phosphate dealkylation activity of boron bromide Schiff base acidic binuclear chelates)

RN 570414-19-6 CAPLUS

CN Boron, tetrabromo[μ-[[2,2'-[1,6-hexanediylibis[(nitrilo-κN)methylidyne]]bis[4,6-bis(1,1-dimethylethyl)phenolato-κO]](2-)]]]di- (9CI) (CA INDEX NAME)

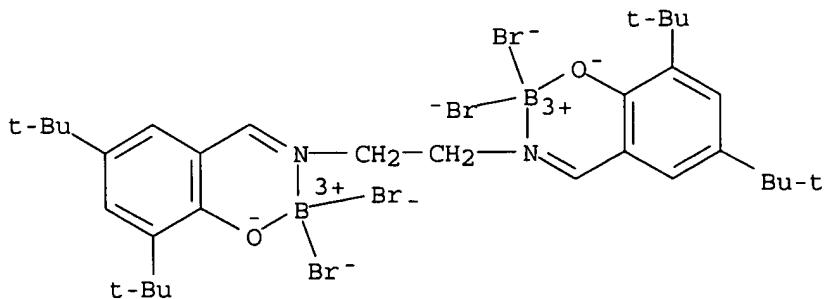


IT 570414-18-5P

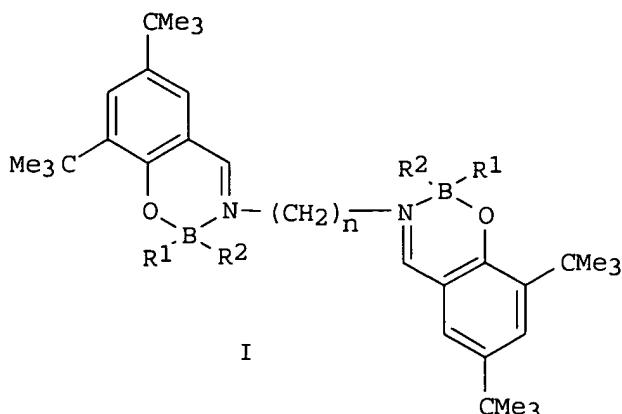
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (phosphate dealkylation; preparation, structure and phosphate dealkylation activity of boron bromide Schiff base acidic binuclear chelates)

RN 570414-18-5 CAPLUS

CN Boron, tetrabromo[μ-[[2,2'-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[4,6-bis(1,1-dimethylethyl)phenolato-κO]](2-)]]]di- (9CI) (CA INDEX NAME)



GI



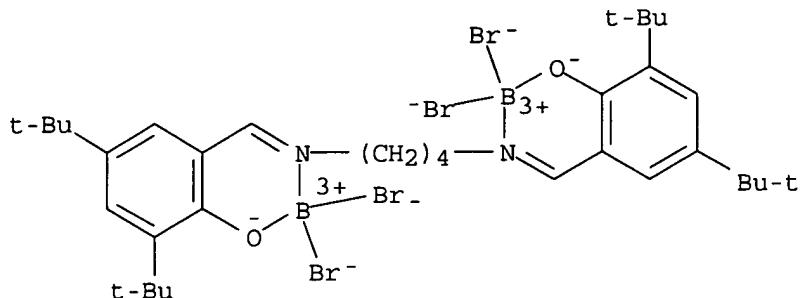
AB Potential two-center Lewis acid compds., bis-salicylimine boron bromide complexes, were prepared and their activity in phosphate dealkylation reaction was examined Compds. (I) (1-6; 1, 2: R₁ = R₂ = Br, N = 2, 6; 3-6: R₁ = p-tolyl, R₂ = Br, n = 2, 3, 4, 6) were prepared by BBr₃ bromination of corresponding methoxy-precursors (I, R₁ = R₂ = OMe or R₁ = p-tolyl, R₂ = OMe). Mono-chelate dibromo[2,4-di-tert-butyl-2-(tert-butylimino)methylphenolato-O,N]boron (7) was also prepared from corresponding dimethoxy-complex. These compds. are active towards the dealkylation of alkyl phosphates and are catalytic when stoichiometric amts. of BBr₃ and tri-Me phosphate are introduced to the chelate ligand. All of the compds. were characterized ¹H- and ¹¹B-NMR, IR, MS; x-ray crystal structure of 2 is reported.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2002:106412 CAPLUS
 DOCUMENT NUMBER: 136:309952
 TITLE: Catalytic Dealkylation of Phosphates with Binuclear Boron Compounds
 AUTHOR(S): Keizer, Timothy S.; De Pue, Lauren J.; Parkin, Sean; Atwood, David A.
 CORPORATE SOURCE: Department of Chemistry, University of Kentucky, Lexington, KY, 40506-0055, USA
 SOURCE: Journal of the American Chemical Society (2002), 124(9), 1864-1865
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:309952
 IT 412014-89-2P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and crystal structure of)
 RN 412014-89-2 CAPLUS
 CN Boron, tetrabromo[μ-[[2,2'-[1,4-butanediylbis[(nitrilo-κN)methylidyne]]bis[4,6-bis(1,1-dimethylethyl)phenolato-κO]](2-)]di-, compd. with methylbenzene (1:2) (9CI) (CA INDEX NAME)

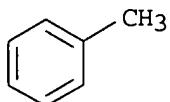
CM 1

CRN 412014-87-0
 CMF C34 H50 B2 Br4 N2 O2
 CCI CCS

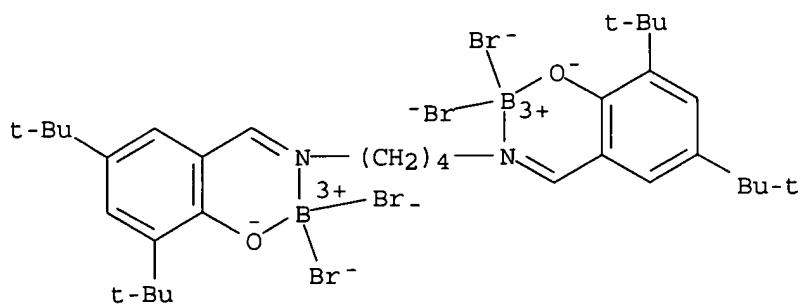


CM 2

CRN 108-88-3
 CMF C7 H8



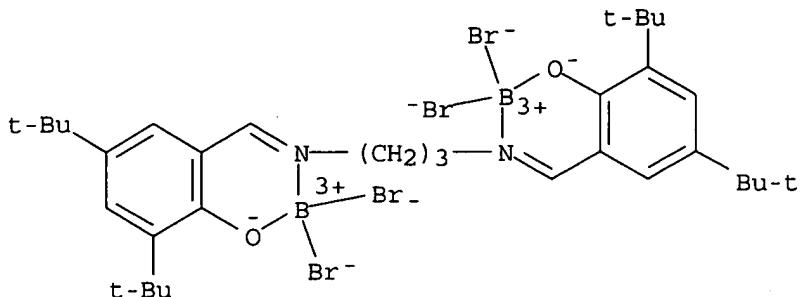
IT 412014-87-0P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and mol. structure of)
 RN 412014-87-0 CAPLUS
 CN Boron, tetrabromo[μ-[[2,2'-[1,4-butanediylbis[(nitrilo-
 κN)methylidyne]]bis[4,6-bis(1,1-dimethylethyl)phenolato-κO]] (2-
)]]di- (9CI) (CA INDEX NAME)



IT 412014-86-9P
 RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation, catalyst for dealkylation of phosphates, and reactivity of)
 RN 412014-86-9 CAPLUS
 CN Boron, tetrabromo[μ-[[2,2'-[1,3-propanediylbis[(nitrilo-
 κN)methylidyne]]bis[4,6-bis(1,1-dimethylethyl)phenolato-κO]] (2-

10/774,619

)]])di- (9CI) (CA INDEX NAME)



AB The Salen(tBu) (*N,N'*-propylenebis(3,5-di-tert-butyl(2-hydroxy)benzylidenimine)) ligand and its derivs. were used to prepare binuclear boron complexes. These compds. have the formula, L(BBr₂)₂ (L = Salpen(tBu) and Salben(tBu) (*N,N'*-butylenebis(3,5-di-tert-butyl(2-hydroxy)benzylidenimine))). These are formed from the reaction of the corresponding L[B(OMe)₂]₂ with BBr₃. They represent a new type of binuclear boron compound. These compds. are active toward the dealkylation of many phosphates. Thus, (OMe)₃P(O) is ~89% dealkylated in the presence of Salpen(tBu)(BBr₂)₂. They are also catalytically active with a stoichiometric amount of BBr₃ to trimethylphosphate.

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT.

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NEWS 18 MAY 23 REGISTRY has been enhanced with source information from CHEMCATS
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NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

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FULL ESTIMATED COST

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| 0.21 | 0.21 |

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FILE COVERS 1907 - 30 Jun 2005 VOL 143 ISS 1
FILE LAST UPDATED: 29 Jun 2005 (20050629/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s chelated borate or borate chelate
9034 CHELATED
61383 BORATE
10673 BORATES
65473 BORATE
(BORATE OR BORATES)
3 CHELATED BORATE
(CHELATED(W) BORATE)
61383 BORATE
10673 BORATES
65473 BORATE
(BORATE OR BORATES)
42713 CHELATE
26602 CHELATES
56625 CHELATE
(CHELATE OR CHELATES)
29 BORATE CHELATE
(BORATE(W) CHELATE)
L1 32 CHELATED BORATE OR BORATE CHELATE

=> s l1 and (halide or halogen or astatine)
148057 HALIDE
123372 HALIDES
214911 HALIDE
(HALIDE OR HALIDES)
103635 HALOGEN
21028 HALOGENS
114256 HALOGEN
(HALOGEN OR HALOGENS)
1587 ASTATINE
2 ASTATINES
1587 ASTATINE
(ASTATINE OR ASTATINES)
L2 0 L1 AND (HALIDE OR HALOGEN OR ASTATINE)

10/774,619

=> s chelate

42713 CHELATE
26602 CHELATES
L3 56625 CHELATE
(CHELATE OR CHELATES)

=> s 13 and (boron or aluminum or gallium or indium or tellurium)

214396 BORON
263 BORONS
214479 BORON
(BORON OR BORONS)
880570 ALUMINUM
297 ALUMINUMS
880632 ALUMINUM
(ALUMINUM OR ALUMINUMS)
281184 GALLIUM
19 GALLIUMS
281184 GALLIUM
(GALLIUM OR GALLIUMS)
181489 INDIUM
11 INDIUMS
181492 INDIUM
(INDIUM OR INDIUMS)
45890 TELLURIUM
14 TELLURIUMS
45893 TELLURIUM
(TELLURIUM OR TELLURIUMS)

L4 4809 L3 AND (BORON OR ALUMINUM OR GALLIUM OR INDIUM OR TELLURIUM)

=> s 14 and (halide or halogen or astatine or flurine or chlorine or bromine or iodine)

148057 HALIDE
123372 HALIDES
214911 HALIDE
(HALIDE OR HALIDES)
103635 HALOGEN
21028 HALOGENS
114256 HALOGEN
(HALOGEN OR HALOGENS)
1587 ASTATINE
2 ASTATINES
1587 ASTATINE
(ASTATINE OR ASTATINES)
13 FLURINE
124254 CHLORINE
758 CHLORINES
124742 CHLORINE
(CHLORINE OR CHLORINES)
49140 BROMINE
158 BROMINES
49237 BROMINE
(BROMINE OR BROMINES)
127621 IODINE
194 IODINES
127695 IODINE
(IODINE OR IODINES)

L5 281 L4 AND (HALIDE OR HALOGEN OR ASTATINE OR FLURINE OR CHLORINE OR BROMINE OR IODINE)

10/774,619

=> s 15 and (ssalen or salpen or salben or salhen)
0 SSALEN
21 SALPEN
15 SALBEN
5 SALHEN
L6 1 L5 AND (SSALEN OR SALPEN OR SALBEN OR SALHEN)

=> s 15 and salen
2669 SALEN
41 SALENS
2676 SALEN
(SALEN OR SALENS)

L7 1 L5 AND SALEN

=> dup rem 16 17
PROCESSING COMPLETED FOR L6
PROCESSING COMPLETED FOR L7
L8 1 DUP REM L6 L7 (1 DUPLICATE REMOVED)

=> d 18 ibib hitstr abs

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2003:18368 CAPLUS
DOCUMENT NUMBER: 138:330730
TITLE: **Boron halide chelate**
compounds and their activity towards the demethylation
of trimethylphosphate
AUTHOR(S): Keizer, Timothy S.; De Pue, Lauren J.; Parkin, Sean;
Atwood, David A.
CORPORATE SOURCE: Department of Chemistry, University of Kentucky,
Lexington, KY, 40506-0055, USA
SOURCE: Canadian Journal of Chemistry (2002), 80(11),
1463-1468
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:330730
AB Salen(t-Bu)H₂ N,N'-ethylenebis(3,5-di-tert-butyl(2-
hydroxy)benzylideneimine) and its derivs. were used to prepare B compds.
L(BCl₂)₂ (L = salen(t-Bu) (1), salpen(t-Bu) (2), salben
(t-Bu) (3), salpten(t-Bu) (4), salhen(t-Bu) (5)). These are
formed from the reaction of the corresponding L[B(OMe)₂]₂ with BC₁₃. In
addition to being a new type of B compound, they are also potential two-point
Lewis acids. Indeed, they demonstrate Lewis acidic behavior in the
dealkylation of trimethylphosphate. All of the compds. were characterized
by m.p., elemental anal., ¹H and ¹¹B NMR, IR, MS, and in the case of 2 by
x-ray crystallog.
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y
COST IN U.S. DOLLARS SINCE FILE TOTAL
SESSION
FULL ESTIMATED COST 57.10 57.31
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

10/774,619

| | | |
|---------------------|----------------|------------------|
| CA SUBSCRIBER PRICE | ENTRY
-0.73 | SESSION
-0.73 |
|---------------------|----------------|------------------|

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